

Hamiltonian Oracles

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Hamiltonian oracles are the continuum limit of the standard unitary quantum oracles. In this limit, the problem of finding the optimal query algorithm can be mapped into the problem of finding shortest paths on a manifold. The study of these shortest paths leads to lower bounds of the original unitary oracle problem. A number of example Hamiltonian oracles are studied in this paper, including oracle interrogation and the problem of computing the XOR of the hidden bits. Both of these problems are related to the study of geodesics on spheres with non-round metrics. For the case of two hidden bits a complete description of the geodesics is given. For n hidden bits a simple lower bound is proven that shows the problems require a query time proportional to n , even in the continuum limit. Finally, the problem of continuous Grover search is reexamined leading to a modest improvement to the protocol of Farhi and Gutmann.

I. INTRODUCTION

As a physical theory quantum mechanics distinguishes itself from its classical counterpart by discretizing certain quantities that were previously considered continuous. Ironically, it is classical computation that is inherently a discrete problem, whereas quantum computation involves a continuous evolution of the state. Nevertheless, when both computational models are extended to include oracles, the queries are introduced as discrete events. While there are good physical reasons for such an oracle model, one is tempted to ask what would constitute half a query to an oracle. For a standard quantum oracle that applies phases of 1 and -1 , half an oracle call could be an application of the phases 1 and i respectively. Surely, two calls to the second oracle are at least as powerful as one call to the standard oracle. Continuing along these lines, one could envision a fraction Δ of an oracle query that applies phases 1 and $e^{i\pi\Delta}$ respectively. If $1/\Delta$ is an integer, then that many calls to this new oracle would be at least as good as one standard oracle query.

Taking the limit $\Delta \rightarrow 0$ one arrives at the Hamiltonian oracle model, first described by Farhi and Gutmann [1]. Roughly speaking, the evolution in this model is given by the Schrödinger equation

$$\frac{d}{dt}|\psi(t)\rangle = -i(H_j + H'(t))|\psi(t)\rangle, \quad (1)$$

where H_j is the Hamiltonian oracle that depends on some hidden parameter j , and $H'(t)$ is a time dependent Hamiltonian that can be chosen arbitrarily but independently of j . The goal of the problem is to evolve from some fixed initial state to a state that contains some information of the hidden parameter j .

The ability to control H' is equivalent to setting $H' = 0$ but being able to apply fast unitaries as often as one wishes. The standard oracle model is simply the restriction that unitaries can be applied only at discrete time

intervals. Therefore, from the perspective of the time evolution of the Gram matrix, continuous oracle algorithms appear as smooth curves whereas algorithms for the equivalent discrete oracles are piece-wise continuous approximations of such curves. The question we ask here is: wouldn't it be easier to study the smooth curves?

This question is in the spirit of recent work by Nielsen et al. [2, 3] which proposes a similar approach to the study of quantum circuit lower bounds. The idea is that differential equations are often easier to solve than difference equations, and that many problems become simpler in the continuum limit.

Given that Hamiltonian oracles can be obtained as the limit $\Delta \rightarrow 0$ of discrete oracles, most of the standard techniques [4, 5, 6] for studying discrete oracles can be used to obtain bounds on Hamiltonian oracles. However, our goal is not to import bounds from the discrete case into the continuous case. Rather we seek to solve Hamiltonian oracle problems by new methods that are intrinsically continuous, and in some cases geometric, and then export these results back into the realm of discrete oracle problems in order to prove new lower bounds. So long as the normalization of the Hamiltonian is chosen so that the continuous oracle equals $O = e^{-iH}$, the minimum query time needed to solve the continuous case will be a lower bound on the number of oracle calls needed to solve the discrete case.

Of course, it is not a priori clear that the continuum limit offers any simplifications. The reductions of both Ref. [2] and the present paper map difficult computer science problems into the problem of finding shortest curves on manifolds, which is also considered a difficult problem. Unfortunately, no new bounds on discrete oracles will be obtained in this paper. Rather, we shall examine Hamiltonian oracles for three problems that have been solved in the discrete case: Oracle interrogation, the problem of computing XOR, and one-item Grover search. However, these examples will serve as an illustration of both the potential that Hamiltonian oracles present and some of the techniques that can be used to exploit them.

Oracle interrogation is the problem where the hidden parameter is an n -bit string which can be queried one

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bit at a time, and we wish to determine the full hidden string. Though n queries are required to solve the problem exactly in the discrete setting, van Dam [7] proved that $n/2 + O(\sqrt{n})$ queries are sufficient to guess the string with very high probability.

In Section IV we show that the continuous version of oracle interrogation can be reduced to the study of shortest curves on S^n with a special metric. For $n = 2$ the metric in polar coordinates can be written as

$$ds^2 = \frac{4}{\pi^2} (d\theta^2 + \tan^2 \theta d\phi^2), \quad (2)$$

and the minimum query time needed to solve the problem exactly is equal to the shortest distance between the points with $\theta = \pi/2$, $\phi = 0$ and $\theta = \pi/4$, $\phi = \pi/4$. We show that a complete set of geodesics can be constructed for this metric, and that the minimum query time for zero error is about 90% of the time required to query both bits separately. This is in contrast with the discrete case where exact solutions never allow any speedup.

For $n > 2$ the metric on S^n is no longer Riemannian but rather of the more general Finsler type. Though the minimal length curves will not be constructed for these cases, we prove in Section IV H a simple lower bound on the query time

$$T \geq \frac{n}{\pi e} + \Omega(1) \simeq 0.117n \quad (3)$$

which applies to the XOR problem (and hence also to oracle interrogation) in the bounded error setting. This is an important bound, for if the Hamiltonian model were significantly faster than the discrete model at solving oracle interrogation then it would likely be useless for proving good lower bounds.

The one-item Grover search oracle is studied in Section III. It is a simple enough problem that we can observe the transition from the discrete to the continuum limit. Given the ability to apply unitaries only at intervals of length Δ , the problem can be solved exactly in a query time of

$$T = \Delta \left[\frac{\arccos \frac{1}{\sqrt{N}}}{\arcsin \frac{2 \sin(\pi\Delta/2) \sqrt{N-1}}{N}} \right] \quad (4)$$

which implies that for large N we obtain a speedup by a factor of $\Delta / \sin(\pi\Delta/2)$ relative to the standard discrete oracle $\Delta = 1$. The result can be extended to fixed error, and in every case half of the above time is needed to solve the problem with probability greater than one half.

In the continuum limit we obtain a query time

$$T = \frac{1}{\pi} \frac{N}{\sqrt{N-1}} \arccos \frac{1}{\sqrt{N}} \simeq \frac{1}{2} \sqrt{N} - \frac{1}{\pi} + O\left(\frac{1}{\sqrt{N}}\right) \quad (5)$$

for an exact solution, which we prove optimal. The above solution is shorter asymptotically by an additive constant of $-1/\pi$ than the one found by Farhi and Gutmann [1].

Though the difference is irrelevant from a practical perspective, the nature of the different solutions is interesting, and is discussed in Section III E. A similar improvement for the case $N = 2$ was found in Ref. [8].

The analysis technique used in this paper is presented in Section II and is a variant on the adversary and semidefinite programming approaches [4, 6], where we study the evolution of the Gram matrix and use symmetrization to simplify the problem. The problems considered herein are sufficiently symmetric that this technique works well. It also has the benefit that it allows the continuous and discrete problems to be studied together using the same notation. The divergence between the two formulations can be delayed until the last step where we consider the dynamics of the Gram matrix.

We note that it does not appear that there is a unique canonical Hamiltonian for a given unitary oracle. In Section II A we show a pair of unitary oracles that are computationally equivalent, but lead to different Hamiltonian oracles under the process of replacing ones with 0 and minus ones with π . This process also has the undesired effect that it breaks complex conjugation symmetry. An alternative way of obtaining a Hamiltonian is to double the query space and replace a one eigenvalue by two 0's and a minus one eigenvalue by π and $-\pi$. This essentially introduces an ‘‘arrow of time’’ qubit that allows the choice between the canonical evolution and its complex conjugate. In fact, it is this form of oracle that is analyzed in the oracle interrogation and XOR problems as we want to ensure that the lower bounds apply to the most general case. For the Grover search problem the standard oracle was used.

The philosophy that has been adopted in this paper is that Hamiltonian oracles are a tool in the study of the standard discrete oracles. Being able to identify a Hamiltonian (possibly from a given set of Hamiltonians) is also an important problem in experimental physics where the hidden parameter is some physical constant which we are interested in measuring [8]. However, the two problems are somewhat different. The Hamiltonians that correspond to standard unitary oracles typically couple $O(\log n)$ qubits, where n is the number of possible different queries. Such couplings are generally not found in nature. Furthermore, the computational version of the problem only concerns itself with one resource: query time. In the experimental version of the problem one may also need to place bounds on the maximum energy of the control Hamiltonian, how quickly it can be changed and what complexity can be achieved. Balancing these competing resources, however, is beyond the scope of this paper.

In the end, all the Hamiltonian oracles studied in this paper were equivalent up to a constant factor to their discrete counterpart. It is unclear if such a relationship holds in general and if so, how large can this constant be? Future work will have to address this question along the road to finding new lower bounds from Hamiltonian oracles.

Prior work

The first paper to study Hamiltonian oracles from a quantum computation perspective is the work of Farhi and Gutmann [1] as discussed above.

The paper by Fenner [9] reexamines the continuous Grover search with a goal of finding a Hamiltonian that matches the discrete case step by step. However, in their construction they allow a total Hamiltonian that is a commutator of the oracle and control Hamiltonians, whose physical motivation is unclear.

The paper by Roland and Cerf [10] also compares the discrete and continuous version of Grover search and studies the simulation of the continuous algorithm by a discrete quantum computer.

Most of the subsequent work involving Hamiltonian oracles studied the problem of spatial search [11, 12], which is a variant of Grover search where the database has some spatial arrangement and only local moves are permitted. The algorithms for these problems employ the continuous quantum walk [13].

There are also many papers that study the problem of identifying a Hamiltonian, though their goals are generally different from ours. For instance, Ref. [14] studies the time-energy uncertainty relation as applied to Hamiltonian identification whereas Ref. [15] shows that in principle a set of Hamiltonians can be distinguished, though the efficiency is not considered. The relation between Hamiltonian oracles and identifying Hamiltonians in the laboratory was also discussed above: Childs, Preskill and Renes [8] continued the work on Hamiltonian oracles, with a view towards exporting the knowledge of quantum computation to the realm of experimental physics. In the same spirit is the work of quantum parameter estimation for dynamical systems, such as the paper by Mabuchi [16].

Finally, the study of Hamiltonian oracles can be recast into a number of formalisms including time optimal control [17] which also greatly benefits from geometric approaches. As a Hamiltonian oracle problem can be studied as a single bipartite Hamiltonian where one can perform arbitrary operations on one side only, this can be translated into the language of optimal control by identifying the oracle Hamiltonian as a drift Hamiltonian, and the subgroup of allowed operations $K \subset G$ as those that act on only one subsystem. Once again, however, the typical Hamiltonians that are of interest in one field are fairly different from those of the other.

II. MODELS AND METHODS

Below we shall introduce a more formal definition of the Hamiltonian oracle model, which will be presented in a language that emphasizes its connections to discrete oracles. We shall use the description of oracle problems as an Alice-Bob game, with Alice taking the place of the oracle. This will facilitate the translation of the prob-

lem into a semidefinite program using Kitaev's construction for coin-flipping [18]. The resulting semidefinite program will be equivalent to the one of Barnum, Saks and Szegedy [6], though it will be easier to symmetrize. Most of the discussion in this section has appeared elsewhere and is intended mainly for review purposes and to fix the notation used for the rest of the paper.

In the Alice-Bob game description of the oracle problem Alice starts with a hidden string (or superposition of strings) in a Hilbert space \mathcal{A} . Bob can query Alice by sending a message in some space \mathcal{M} . Alice always applies some known fixed unitary (or Hamiltonian) to $\mathcal{A} \otimes \mathcal{M}$ and returns \mathcal{M} to Bob. Of course, Bob is allowed to have his own private Hilbert space \mathcal{B} , however it will never be explicitly referenced as everything will be described from Alice's perspective.

In the end Bob must guess some property of the hidden string, and send his guess to Alice in space \mathcal{M}' , who determines whether it is correct or not. We say that Bob wins when Alice accepts his answer, and the goal is to maximize this probability.

In principle, given a strategy for Bob, we need to try it against each of the possible hidden strings, one at a time. Because we are interested in the worse-case success probability, we take the minimum over the success probabilities for the different possible hidden strings. However, as is common in adversary methods, Alice can start with a superposition over different possible input strings. In such a case the worse-case success probability can be calculated by a single run through the Alice-Bob game. However, the operation which computes this final worse-case success probability is not a physical quantum measurement but rather just a linear expression involving Alice's final density operator. Nevertheless, it will be Bob's goal to use his interactions with Alice in order to attain a final density operator that maximizes the expression for the success probability. We shall say more about this final operation below.

Formally, we define an oracle problem by three Hilbert spaces \mathcal{A} , \mathcal{M} and \mathcal{M}' , together with an initial pure state $|\psi_0\rangle$ on \mathcal{A} , a unitary operator O (or Hermitian operator H in the continuous case) on $\mathcal{A} \otimes \mathcal{M}$, and a set of positive operators $\{\Pi_x\}$ on $\mathcal{A} \otimes \mathcal{M}'$ labeled by an index x which usually ranges over the set of hidden strings. For the discrete case we also specify a positive number Δ corresponding to an interval of time.

A protocol for an oracle problem is given by a positive time T (divisible by Δ in the discrete case), a success probability P_{win} , a pair of functions $\rho(t)$ and $\tilde{\rho}(t)$ for $0 \leq t \leq T$ (valued at integer multiples of Δ for the discrete case) and a final matrix $\tilde{\rho}'$. We require that $\rho(t)$, $\tilde{\rho}(t)$ and $\tilde{\rho}'$ be positive operators on the spaces \mathcal{A} , $\mathcal{A} \otimes \mathcal{M}$ and $\mathcal{A} \otimes \mathcal{M}'$ respectively. They must satisfy the following equations:

- Initialization:

$$\rho(0) = |\psi_0\rangle\langle\psi_0|_{\mathcal{A}}. \quad (6)$$

- Bob's action (for $0 \leq t \leq T$):

$$\text{Tr}_{\mathcal{M}}[\tilde{\rho}(t)] = \rho(t). \quad (7)$$

- Alice's action

- for discrete time ($0 \leq t \leq T - \Delta$)

$$\rho(t + \Delta) = \text{Tr}_{\mathcal{M}}[O\tilde{\rho}(t)O^{-1}]. \quad (8)$$

- for continuous time ($0 \leq t \leq T$)

$$\frac{d}{dt}\rho(t) = -i \text{Tr}_{\mathcal{M}}[H\tilde{\rho}(t) - \tilde{\rho}(t)H]. \quad (9)$$

- Bob's output:

$$\text{Tr}_{\mathcal{M}'}[\tilde{\rho}'] = \rho(T). \quad (10)$$

- Answer verification (for every x):

$$P_{win} \leq \text{Tr}[\Pi_x \tilde{\rho}']. \quad (11)$$

A standard discrete-time oracle problem will have $\Delta = 1$, however, the above formulation allows us to pass to the continuous time limit by defining $O = e^{-i\Delta H}$ and then taking the limit $\Delta \rightarrow 0$.

The basic goal of the problem is to choose the protocol $\rho(t)$, $\tilde{\rho}(t)$ and $\tilde{\rho}'$ as to maximize the probability of winning P_{win} , for a given time T . Of course, eventually one wants to invert the relation: fix P_{win} and find the smallest T for which it can be achieved as a function of some scaling of the problem.

The above formulation should be understood as follows: Say Alice has a density operator $\rho(t)$ on \mathcal{A} at a given time t . When Bob queries Alice by sending a message in the space \mathcal{M} , Alice ends up with a density operator $\tilde{\rho}(t)$ on the larger space $\mathcal{A} \otimes \mathcal{M}$. This operator must satisfy the consistency condition given by Eq. (7) because Bob cannot affect the state of \mathcal{A} . Having received Bob's message, Alice applies the oracle operation and returns \mathcal{M} to Bob, ending up with a new state defined by Eq. (8) or Eq. (9).

To relate the above definition to the standard oracle model we let \mathcal{A} be the Hilbert space spanned by the set of hidden strings. Then $O = \sum_x |x\rangle\langle x|_{\mathcal{A}} \otimes O_x$ where O_x are the standard oracle operators on \mathcal{M} given hidden parameter x . For the continuous case we similarly have $H = \sum_x |x\rangle\langle x|_{\mathcal{A}} \otimes H_x$.

A good guess for the final operation would be the two-outcome POVM $\{\Pi, I - \Pi\}$, where $\Pi = \sum_x |x\rangle\langle x|_{\mathcal{A}} \otimes |f(x)\rangle\langle f(x)|_{\mathcal{M}'}$ and $f(x)$ is the target function to compute such as XOR. We would then declare Bob a winner only if the first outcome was obtained, thereby setting $P_{win} = \text{Tr}[\Pi \tilde{\rho}']$. However, this only computes the average success probability rather than the worse-case success probability. Instead, the correct prescription is to use Eq. (11) with $\Pi_x = |x\rangle\langle x|_{\mathcal{A}} \otimes |f(x)\rangle\langle f(x)|_{\mathcal{M}'} / |\langle x|\psi_0\rangle|^2$, so that $\text{Tr}[\Pi_x \tilde{\rho}']$ will be the probability of Bob correctly answering given that the hidden string was x .

For the discrete oracle case deriving the above semidefinite program is fairly simple. Clearly no matter what actions Bob performs, Alice's density operators must satisfy the above equations. On the other hand, because Alice starts with a pure state and makes no measurements, Bob can keep the purification of Alice's state and therefore force any evolution consistent with the above equations.

To arrive at the continuous case simply define $\Delta = 2^{-k}$ and $O = e^{-i\Delta H}$ for $k \in \mathbb{Z}^+$. Given some fixed T , let $P_{win}(k)$ be the maximum over all protocols for the discrete oracle problem with a given k . Trivially, $P_{win}(k+1) \geq P_{win}(k)$. If we also defined the problem so that $P_{win}(k) \leq 1$ for all k , then in the limit $k \rightarrow \infty$ we converge to a well defined $P_{win}(\infty)$. This can be taken as a formal definition of the Hamiltonian oracle problem. In this limit we can replace the discrete evolution with the continuous evolution given by Eq. (9), so long as we restrict $\tilde{\rho}(t)$ to be continuous (or more generally measurable if we use the integral form of the equation).

The more traditional definition of a Hamiltonian oracle is that there is a set of Hamiltonians $\{H_x\}$ acting on a space \mathcal{M} . Bob can append a set of extra qubits with the space \mathcal{B} on which the Hamiltonians act trivially. He can then control the system by either adding an extra Hamiltonian H' , by periodically applying unitary operators, or by conjugating $H_x \otimes I_{\mathcal{B}}$ by some time dependent unitary of his choosing, so long as these operations don't depend on the hidden parameter x . These three variants are all equivalent, and equivalent to the model where all three activities can be done simultaneously. Though proving the equivalence of these models is beyond the scope of this paper, it is not hard to see that the above continuous SDP serves as a lower bound for all the models, again by the argument that no matter what Bob does, the qubits in Alice's possession are restricted to evolve according to the above equations.

We note in closing that the above SDP can be separated into two problems: The first is finding the set of attainable final density operators $\rho(T)$. The second problem involves finding the optimal $\tilde{\rho}'$ and maximal P_{win} given $\rho(T)$. Solving the second problem is often easy, leading to a function $P_{win}(\rho(T))$. Therefore, most of the effort below will involve searching for the evolution towards a good final density operator $\rho(T)$.

A. On canonical Hamiltonians

In this section we shall examine an oddity that arises in the transition from discrete to continuous oracles. Clearly given an oracle unitary, O , there are infinitely many Hamiltonians H such that $O = e^{-iH}$. However, if O is a standard oracle with only eigenvalues 1 and -1 then a canonical Hamiltonian can be defined by the process of replacing the one eigenvalues by 0 and the minus one eigenvalues by π .

Unfortunately, while the above mapping does associate

a unique Hamiltonian to each unitary oracle, there are cases when unitary oracles of equivalent computational power are mapped into Hamiltonians of different computational power.

Consider for instance the oracle with a hidden bit $b \in \{0, 1\}$, and the two unitary oracles

$$O_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad O_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad (12)$$

where the complete oracle in the notation of the previous section would be $O = |0\rangle\langle 0|_{\mathcal{A}} \otimes O_0 + |1\rangle\langle 1|_{\mathcal{A}} \otimes O_1$. A different pair of oracles for the same problem are given by

$$O'_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad O'_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (13)$$

with O' defined similarly. The two pairs of oracles are clearly equivalent, as one can simulate one with the other by simply applying a phase flip to the third basis state.

Now consider the Hamiltonians obtained from the above unitaries by the standard eigenvalue replacement

$$H_0 = \pi \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad H_1 = \pi \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (14)$$

and

$$H'_0 = \pi \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad H'_1 = \pi \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (15)$$

where again $H = |0\rangle\langle 0|_{\mathcal{A}} \otimes H_0 + |1\rangle\langle 1|_{\mathcal{A}} \otimes H_1$ and similarly for H' . With the first oracle pair it takes one unit of time to perfectly distinguish between the two Hamiltonians, whereas with the second pair only half a unit of time is required.

In general, the existence of many choices for the Hamiltonian oracle is not a problem. So long as the normalization is chosen so that e^{-iH} is computationally equivalent to the discrete oracle that needs lower bounding, one may choose any Hamiltonian that is easy to study.

B. Reduction by preponderance of symmetry

In the next two sections we shall show how oracle problems with large amounts of symmetry can be simplified because they always have an optimal solution that shares the symmetry of the problem, and therefore the search for the optimal solution can be conducted over the smaller space of density operators that are invariant under the action of the symmetry group.

We say that a group G is compatible with an oracle problem $|\psi_0\rangle$, O (or H for the continuous case), and $\{\Pi_x\}$

if there exists unitary representations $R_{\mathcal{A}}$ on \mathcal{A} , $R_{\mathcal{M}}$ on \mathcal{M} and $R_{\mathcal{M}'}$ on \mathcal{M}' such that for all $g \in G$ we have

$$R_{\mathcal{A}}(g)|\psi_0\rangle = |\psi_0\rangle, \quad (16)$$

$$R(g)OR(g^{-1}) = O, \quad (17)$$

$$R(g)HR(g^{-1}) = H, \quad (18)$$

$$\{R'(g)\Pi_x R'(g^{-1})\} = \{\Pi_x\}, \quad (19)$$

where for simplicity we have introduced $R(g) = R_{\mathcal{A}}(g) \otimes R_{\mathcal{M}}(g)$ and $R'(g) = R_{\mathcal{A}}(g) \otimes R_{\mathcal{M}'}(g)$. In the last equation, the symmetry does not need to leave the operators Π_x element-wise invariant, but must leave the set invariant.

Given a solution $\tilde{\rho}(t)$ to a G compatible oracle problem, we can define for $g \in G$

$$\tilde{\rho}_g(t) = R(g)\tilde{\rho}(t)R(g^{-1}) \quad (20)$$

for $t \in [0, T]$ and similarly

$$\tilde{\rho}'_g = R'(g)\tilde{\rho}'R'(g^{-1}), \quad (21)$$

which will be solutions to the oracle problem with the same success probability (as can easily be verified). Naturally, the reduced density operator on Alice's side will be $\rho_g(t) = \text{Tr}[\tilde{\rho}_g(t)] = R_{\mathcal{A}}(g)\rho(t)R_{\mathcal{A}}(g^{-1})$.

Because the equations are all linear, we can also take linear combinations of solutions. Given a solution $\tilde{\rho}(t)$ define

$$\tilde{\rho}_G(t) = \frac{1}{|G|} \sum_{g \in G} \tilde{\rho}_g(t) \quad (22)$$

and similarly for $\tilde{\rho}'_G$. These must also be a solution of the oracle problem with the same success probability as $\tilde{\rho}(t)$ and $\tilde{\rho}'$. Note that this is a non-vanishing solution because $\tilde{\rho}(t) = 0$ cannot be a solution of the equations. In fact, the equations impose conservation of trace so that for all t we have $\text{Tr}[\tilde{\rho}_G(t)] = \langle \psi_0 | \psi_0 \rangle$.

We call a solution G -invariant if for all $g \in G$ and $t \in [0, T]$ it satisfies $R(g)\tilde{\rho}(t)R(g^{-1}) = \tilde{\rho}(t)$, and furthermore $R'(g)\tilde{\rho}'R'(g^{-1}) = \tilde{\rho}'$ again for all $g \in G$. A G invariant solution will also imply that $R_{\mathcal{A}}(g)\rho(t)R_{\mathcal{A}}(g^{-1}) = \rho(t)$ for all $g \in G$ and at all times.

It is not hard to see that given any solution $\tilde{\rho}(t)$, the solution $\tilde{\rho}_G(t)$ constructed from it as above will be G -invariant, and will have the same probability of success. We have therefore proven the following lemma:

Lemma 1. *Given an oracle problem that is compatible with a group G , the set of success probabilities P_{win} that can be achieved with query time T will not be altered if we restrict the space of solutions to those that are G -invariant.*

The lemma allows us to concentrate only on G -invariant solutions when studying both upper and lower bounds.

C. Further reductions for standard oracles

Up to this point the set of allowed oracle unitaries or Hamiltonians has been left unrestricted, but now we shall focus on the standard oracles that change the phase of the states in \mathcal{M} based on the value of the hidden oracle string.

Given a basis $\{|j\rangle_{\mathcal{A}}\}$ for \mathcal{A} and a basis $\{|k\rangle_{\mathcal{M}}\}$ for \mathcal{M} , which we refer to as the computational bases, we say that O or H is in standard form if it can be written as

$$\sum_{j,k} C_{j,k} |j\rangle_{\mathcal{A}} \langle j|_{\mathcal{A}} \otimes |k\rangle_{\mathcal{M}} \langle k|_{\mathcal{M}}, \quad (23)$$

where the coefficients $C_{j,k}$ are real numbers in the case of a Hamiltonian oracle and phases in the case of a unitary oracle.

We further assume that the oracle problem is compatible with a group G and that the action of this group on the space \mathcal{M} is by permutation of the basis:

$$R_{\mathcal{M}}(g)|k\rangle_{\mathcal{M}} = |s(g)k\rangle_{\mathcal{M}} \quad (24)$$

for all k and $g \in G$, where $s(g)$ is a homomorphism from G to the symmetric group S_M and $M = |\mathcal{M}|$. For simplicity we assume here that the index set k ranges from 1 to M so that S_M acts naturally on the index set by permutation. In such a case the symmetry group G can be extended to $G_Q = (\mathbb{Z}_2)^M \rtimes G$, where the semidirect product is defined by $(x', g')(x, g) = (x' \oplus s(g)x, g'g)$ with $x \in (\mathbb{Z}_2)^M$ and M -digit binary string and $s(g') \in S_M$ acting on it by permutation.

We can define representations of G_Q on the spaces \mathcal{A} and \mathcal{M}' by $R_{\mathcal{A}}(x, g) = R_{\mathcal{A}}(g)$ and $R_{\mathcal{M}'}(x, g) = R_{\mathcal{M}'}(g)$. The nontrivial extension is the representation of G_Q on \mathcal{M} defined by

$$R_{\mathcal{M}}(x, g)|k\rangle = (-1)^{x_{s(g)k}} |s(g)k\rangle, \quad (25)$$

where x_k denotes the k th bit of x . It is simple to verify that if the a standard oracle problem is compatible with G , then it will also be compatible with G_Q .

A G_Q -invariant operator $\tilde{\rho}$ on $\mathcal{A} \otimes \mathcal{M}$ must have the block diagonal form

$$\sum_k \sigma_k \otimes |k\rangle_{\mathcal{M}} \langle k|_{\mathcal{M}}, \quad (26)$$

where the σ_k are positive operators on \mathcal{A} . The block diagonalization follows simply by considering the action of group elements of the form $(x, 1)$, where x is a string with a single 1 entry.

The σ_k are further restricted as follows:

- The operators σ_k must be invariant under the stabilizer of k , that is, for all $g \in G$ such that $s(g)k = k$ we must have $R_{\mathcal{A}}(g)\sigma_k R_{\mathcal{A}}(g^{-1}) = \sigma_k$.
- If there exists a g such that $s(g)k = k'$ then $\sigma_{k'} = R_{\mathcal{A}}(g)\sigma_k R_{\mathcal{A}}(g^{-1})$ for any such g .

The condition $s(g)k = k'$ for some $g \in G$ defines an equivalence relationship on the integers $[M]$, and allows us to divide them into equivalence classes. The most general G -invariant $\tilde{\rho}$ can therefore be specified by only one matrix σ_k for each equivalence class, which must be invariant under the stabilizer of k .

Of course, all of the above discussion would be moot if we had just begun with the symmetry group G_Q in the first place. However, in this paper we shall choose G to correspond with the symmetry of the classical problem, and then G_Q will be the extended symmetry that appears in the quantum case.

We conclude this section by noting how the symmetry simplifies density operators ρ on \mathcal{A} (as opposed to $\tilde{\rho}$ on $\mathcal{A} \otimes \mathcal{M}$ as we have been discussing thus far). If the decomposition of the representation $R_{\mathcal{A}}$ into irreducible representations contains at most one copy of each irrep, then by Schur's lemma the most general G -invariant ρ has the form

$$\sum_{\alpha} a_{\alpha}^2 P_{\alpha}, \quad (27)$$

where α ranges over the irreps appearing in $R_{\mathcal{A}}$, P_{α} is the projector onto the irrep, and the a_{α}^2 are non-negative constants that sum to $\langle \psi_0 | \psi_0 \rangle$ which we assume here is one. It will be convenient to deal with the vectors (a_0, a_1, \dots) which specify a point on the unit sphere for some dimension. This point on the sphere will be a complete description of the state of the protocol at a given instant of time, or equivalently, of Bob's knowledge at that instant of time.

III. ONE-ITEM GROVER SEARCH

Here we study the Grover search problem under the promise that exactly one item is marked. The goal, as usual, is to identify the marked item. Though this problem has been extensively studied in the literature, it will provide a good example for the ideas discussed in the previous section, and as a comparison of the discrete and continuous oracle models. Furthermore, we shall find a modest improvement to the protocol found by Farhi and Gutmann [1].

Our strategy below, after defining the problem in the new notation, will be to identify the symmetry group of the problem and use it to reduce the search space of potential solutions. Within this reduced space we will then identify the initial state and the set of final states from which the marked state can be identified with small error. Finally, we study the dynamics needed to evolve from the initial state to these good final states, which will tell us the query time needed to solve the oracle problem. Note that it is only in this last step that the discrete and continuous oracle models need to be handled separately.

A. Problem definition

Fix an integer $N > 1$ and define

$$\mathcal{A} = \text{span}\{|j\rangle \text{ for } j \in [N]\}, \quad (28)$$

$$\mathcal{M} = \mathcal{M}' = \text{span}\{|j\rangle \text{ for } j \in \{0\} \cup [N]\}, \quad (29)$$

and on these spaces we define

$$|\psi_0\rangle = |+\rangle_{\mathcal{A}} \equiv \frac{1}{\sqrt{N}} \sum_{j=1}^N |j\rangle_{\mathcal{A}}, \quad (30)$$

$$H = \pi \sum_{j=1}^N |j\rangle\langle j|_{\mathcal{A}} \otimes |j\rangle\langle j|_{\mathcal{M}}, \quad (31)$$

$$O_{\Delta} = I - (1 - e^{-i\pi\Delta}) \sum_{j=1}^N |j\rangle\langle j|_{\mathcal{A}} \otimes |j\rangle\langle j|_{\mathcal{M}}, \quad (32)$$

$$\Pi_j = N|j\rangle\langle j|_{\mathcal{A}} \otimes |j\rangle\langle j|_{\mathcal{M}}, \quad \text{for } j \in [N]. \quad (33)$$

Note that the normalization of H is chosen so that $O_{\Delta} = e^{-i\Delta H}$, and the unit of time is chosen so that $\Delta = 1$ corresponds to the standard discrete time oracle. In both cases, the query space H has a state $|0\rangle$ which is left invariant by H and O . This is the null query.

The normalization of $|\psi_0\rangle$ to a unit vector, though natural from a quantum mechanical perspective, will imply that Alice's reduced density operator will not be the Gram matrix but rather the Gram matrix scaled by $1/N$. This is also the source of the factor of N in the operators Π_j . After the symmetrization below we will be able to replace the N projectors $\{\Pi_j\}$ with the single projection operator $\Pi = \sum_j \Pi_j/N$ because the worst-case and average-case success probabilities will be equal.

B. Symmetrization

The natural symmetry group for the problem is $G = S_N$ which acts by permutation on \mathcal{A} and on the last N states of \mathcal{M} , but leaves $|0\rangle_{\mathcal{M}}$ invariant. With these definitions the oracle is compatible with the symmetry group.

The most general density matrix ρ on \mathcal{A} which is G -invariant is given by

$$\rho = x|+\rangle\langle +| + y(I - |+\rangle\langle +|). \quad (34)$$

The two parameters are related because we require $x + (N-1)y = \text{Tr}[\rho] = \langle \psi_0 | \psi_0 \rangle = 1$. Therefore ρ (and hence the state of the system at any given time) depends on the single parameter x .

We now turn to the symmetrization of operators $\tilde{\rho}$ on $\mathcal{A} \otimes \mathcal{M}$. As the oracle is of standard form, and the symmetry group acts by permutation on \mathcal{M} , we can apply the results of Section II C. The most general $\tilde{\rho}$ consistent with the symmetries of the problem has the form

$$\tilde{\rho} = \sigma_0 \otimes |0\rangle\langle 0|_{\mathcal{M}} + \sum_{j=1}^N R_{\mathcal{A}}(g_{1,j}) \sigma_1 R_{\mathcal{A}}(g_{1,j}^{-1}) \otimes |j\rangle\langle j|_{\mathcal{M}}, \quad (35)$$

where $g_{1,j}$ is any element that maps 1 to j .

The matrix σ_0 must be invariant under the complete S_N so that its most general form is

$$\sigma_0 = x_0|+\rangle\langle +| + y_0(I - |+\rangle\langle +|), \quad (36)$$

where positivity demands $x_0 \geq 0$ and $y_0 \geq 0$.

On the other hand, the matrix σ_1 need be invariant only under the subgroup S_{N-1} that leaves $|1\rangle_{\mathcal{M}}$ invariant. Under the full S_N we saw that \mathcal{A} decomposes into two irreps: the space spanned by $|+\rangle_{\mathcal{A}}$ and its orthogonal complement. Under the restriction to S_{N-1} , the first representation will naturally still be irreducible, but the second one will decompose into the space spanned by

$$|-1\rangle = \sqrt{\frac{N-1}{N}}|1\rangle - \sqrt{\frac{1}{N(N-1)}} \sum_{j=2}^N |j\rangle \quad (37)$$

and its orthogonal complement, leading to a decomposition of \mathcal{A} into three irreps. However, since the first two are both the trivial representation, Schur's lemma does not prevent them from sharing off-diagonal terms and therefore the most general S_{N-1} invariant operator on \mathcal{A} has the form

$$\sigma_1 = (|+\rangle \quad |-1\rangle) \begin{pmatrix} a & b \\ b^* & c \end{pmatrix} \begin{pmatrix} \langle +| \\ \langle -1| \end{pmatrix} + d P_1^{\perp}, \quad (38)$$

where $P_1^{\perp} = (I - |+\rangle\langle +| - |-1\rangle\langle -1|)$ is the projector onto the orthogonal complement of the space that contains $|+\rangle$ and $|1\rangle$. Positivity of σ_1 requires $a \geq 0$, $c \geq 0$, $d \geq 0$ and $|b|^2 \leq ac$.

To conclude, we compute the partial trace of a given $\tilde{\rho}$ of the above form. It is given by the sum of the projections of σ_i onto the invariant subspaces of the full S_N :

$$\begin{aligned} \text{Tr}_{\mathcal{M}}[\tilde{\rho}] &= (x_0 + aN)|+\rangle\langle +| \\ &+ (y_0 + c \frac{N}{N-1} + d \frac{N(N-2)}{N-1})(I - |+\rangle\langle +|). \end{aligned} \quad (39)$$

C. Boundary conditions

We now proceed to treat ρ , and consequently x , as a function of time. The initial condition at time $t = 0$ is fairly simple $\rho(0) = |\psi_0\rangle\langle \psi_0|$ and hence $x(0) = 1$.

We need to determine what values for $x(T)$ are acceptable as final conditions. The final probability of success P_{win} depends only on $x(T)$. Because of the symmetry of the problem, the optimal measurement is the pretty-good measurement and the success probability is given [19, 20, 21] by

$$\begin{aligned} P_{win}(x(T)) &= \frac{1}{N} \left(\text{Tr} \sqrt{\rho(T)} \right)^2 \\ &= \frac{1}{N} \left(\sqrt{x(T)} + \sqrt{(N-1)(1-x(T))} \right)^2. \end{aligned} \quad (40)$$

In particular, a zero error outcome requires $x(T) = 1/N$. On the other hand $x(T) = 1/2$ implies $P_{win} =$

$1/2 + \sqrt{N-1}/N$, so that a solution with some fixed error $P_{win} > 1/2$ as $N \rightarrow \infty$ requires at a minimum $x(T) < 1/2$.

D. Dynamics

Bob's task is now clear. He must use the dynamics of the system so that x evolves from 1 at time $t = 0$, and decreases as quickly as possible, past $1/2$ for constant error and stopping at $1/N$ for zero error.

1. Continuous time

We begin with the continuous case, with dynamics given by Eq. (9), which leads to a differential equation for $x(t)$:

$$\begin{aligned} \frac{dx(t)}{dt} &= -i\langle + | \text{Tr}_M[H\tilde{\rho}(t) - \tilde{\rho}(t)H] | + \rangle \\ &= -\frac{i\pi}{\sqrt{N}} \sum_{j=1}^N \langle j | \sigma_j(t) | + \rangle - \langle + | \sigma_j(t) | j \rangle \\ &= 2\pi\sqrt{N-1} \text{Im}[b(t)]. \end{aligned} \quad (41)$$

The differential equation for $y(t)$ is uninteresting, as it is related to the above by the normalization condition $x(t) + (N-1)y(t) = 1$.

Bob controls the dynamics via his choice of $\tilde{\rho}(t)$ at each time, which he clearly would like to choose so that the imaginary part of $b(t)$ is as negative as possible. By positivity of $\tilde{\rho}$ we know that $|b(t)|^2 \leq a(t)c(t)$ whereas the constraint $\text{Tr}_M[\tilde{\rho}(t)] = \rho(t)$ translates via Eq. (39) into $x(t) = x_0(t) + a(t)N$ and $y(t) = (1 - x(t))/(N-1) = y_0 + c(t)N/(N-1) + d(t)N(N-2)/(N-1)$. Combining these constraints we see that

$$-\text{Im}[b(t)] \leq \frac{1}{N} \sqrt{x(t)(1-x(t))} \quad (42)$$

with equality clearly achievable. The evolution of $x(t)$ following the optimal protocol is therefore given by

$$\frac{dx(t)}{dt} = -2\pi \frac{\sqrt{N-1}}{N} \sqrt{x(t)(1-x(t))} \quad (43)$$

which is solved by

$$x(t) = \cos^2 \left(\pi \frac{\sqrt{N-1}}{N} t \right), \quad (44)$$

where we have already included the initial condition $x(0) = 1$. Continuous Grover search can therefore be solved exactly in a time

$$T = \frac{1}{\pi} \frac{N}{\sqrt{N-1}} \arccos \frac{1}{\sqrt{N}} \simeq \frac{1}{2} \sqrt{N}, \quad (45)$$

whereas solving with a fixed error greater than one half requires a query time of at least $N/(4\sqrt{N-1})$.

2. Discrete time

For the discrete case we have

$$\begin{aligned} x(t+\Delta) &= \langle + | \text{Tr}_M[O\tilde{\rho}(t)O^{-1}] | + \rangle \\ &= x_0(t) + N \begin{pmatrix} \alpha & \beta \end{pmatrix} \begin{pmatrix} a(t) & b(t) \\ b^*(t) & c(t) \end{pmatrix} \begin{pmatrix} \alpha^* \\ \beta^* \end{pmatrix}, \end{aligned} \quad (46)$$

where

$$\alpha = \langle + | O_1 | + \rangle = 1 - \frac{1 - e^{-i\pi\Delta}}{N}, \quad (47)$$

$$\beta = \langle + | O_1 | -_1 \rangle = -\frac{(1 - e^{-i\pi\Delta})\sqrt{N-1}}{N}, \quad (48)$$

and $O_1 = I - (1 - e^{i\pi\Delta})|1\rangle\langle 1|$ is the oracle operator when query one is issued. Note that $|\alpha|^2 + |\beta|^2 = 1$.

Before solving the general case of the above equation, we must address what happens in the last query. Assume that at some time t we have $x(t) > 1/N$ but for some setting of the parameters we can achieve $x(t+\Delta) \leq 1/N$. Because $x(t+\Delta)$ is continuous in the parameters of $\tilde{\rho}(t)$, and we could have also issued a null query (i.e., setting $a(t) = b(t) = c(t) = d(t) = 0$, $x_0(t) = x(t)$, and $y_0(t) = y(t)$ so that $x(t+\Delta) = x(t)$) there must be a query such that $x(t+\Delta) = 1/N$, and therefore the problem can be solved exactly in $t + \Delta$ queries.

For all other times we know that for any choice of $\tilde{\rho}(t)$ we must have $x(t+\Delta) > 1/N$. In this case Bob simply wishes to make $x(t+\Delta)$ as small as possible. Given that any solution with $x_0(t) > 0$ we can always find a better solution by choosing $x_0(t) = 0$ and $a(t) = x(t)/N$. The only two constraints in which $a(t)$ or $x_0(t)$ appear are $x(t) = x_0(t) + Na(t)$ which is satisfied by the new variables, and $a(t)c(t) \geq |b(t)|^2$ which is also satisfied as we have not decreased $a(t)$.

Similarly, given any assignment of the above variables, we can always set

$$b(t) = -\sqrt{a(t)c(t)} \frac{\alpha^* \beta}{|\alpha\beta|} \quad (49)$$

which will not increase $x(t+\Delta)$. With these simplifications, the optimal solutions must be of the form:

$$x(t+\Delta) = N \left(|\alpha| \sqrt{\frac{x(t)}{N}} - |\beta| \sqrt{c(t)} \right)^2 \quad (50)$$

for some $c(t) \in [0, (1-x(t))/N]$. However, since by assumption $x(t+\Delta)$ cannot be zero, it must be minimized by $c(t) = (1-x(t))/N$. We are left with the recursive relation

$$x(t+\Delta) = \left(|\alpha| \sqrt{x(t)} - |\beta| \sqrt{1-x(t)} \right)^2 \quad (51)$$

which is solved, with starting point $x(0)=1$, by

$$x(t) = \cos^2 \left(\arcsin(|\beta|) \frac{t}{\Delta} \right) \quad (52)$$

yielding an exact solution in a query time

$$T = \Delta \left[\frac{\arccos \frac{1}{\sqrt{N}}}{\arcsin \frac{2 \sin(\pi \Delta/2) \sqrt{N-1}}{N}} \right]. \quad (53)$$

As before a fixed error greater than one half can also be attained in approximately half the time.

E. Discussion

Just as in the discrete case, the optimal continuous protocol for one-item Grover search can be described as a rotation in the two-dimensional subspace that contains the vectors $|+\rangle$ and the marked state $|j\rangle$. This rotation is effectuated by the Hamiltonian

$$H_{total} = H_j + H' = \pi|j\rangle\langle j| + \pi \frac{N-2}{N} |+\rangle\langle +|, \quad (54)$$

where H_j is the oracle Hamiltonian if the hidden string is j , and H' is the j independent Hamiltonian that defines the algorithm. In the orthonormal basis $|+\rangle$ and $|-\rangle$ for the relevant two dimensional subspace the above equation reads

$$\begin{aligned} H_{total} &= \frac{\pi}{N} \left[\begin{pmatrix} 1 & \sqrt{N-1} \\ \sqrt{N-1} & N-1 \end{pmatrix} + \begin{pmatrix} N-2 & 0 \\ 0 & 0 \end{pmatrix} \right] \\ &= \frac{\pi(N-1)}{N} I + \frac{\pi\sqrt{N-1}}{N} \sigma_x, \end{aligned} \quad (55)$$

where $|-\rangle$ is the natural generalization of Eq. (37), and σ_x is the Pauli x operator. The evolution is given by

$$\begin{aligned} |\phi_j(t)\rangle &= e^{-i\pi t(N-1)/N} \left(\cos\left(\frac{\pi t\sqrt{N-1}}{N}\right) |+\rangle \right. \\ &\quad \left. -i \sin\left(\frac{\pi t\sqrt{N-1}}{N}\right) |-\rangle \right) \end{aligned} \quad (56)$$

and at time $T = N/(\pi\sqrt{N-1}) \arccos 1/\sqrt{N}$ we end up (ignoring the global phase) in one of the states

$$|\phi_j(T)\rangle \propto \frac{1}{\sqrt{N}} |+\rangle - i \sqrt{\frac{N-1}{N}} |-\rangle = U|j\rangle, \quad (57)$$

where $U = -iI + (1+i)|+\rangle\langle +|$. At this time all N states become mutually orthogonal, and therefore the N different Hamiltonian oracles can be perfectly distinguished.

In the protocol of Farhi and Gutmann [1], they used oracles of the form $H_j = E|j\rangle\langle j|$, and therefore to compare the results we need to set $E = \pi$. With our notation their total Hamiltonian is given by

$$H_{total} = H_j + H' = \pi|j\rangle\langle j| + \pi|+\rangle\langle +| \quad (58)$$

and after a time of exactly $T = \sqrt{N}/2$ this Hamiltonian will evolve the state $|+\rangle$ into the state $|j\rangle$. This is marginally slower than the optimal time found above

which can be expanded as $\sqrt{N}/2 - 1/\pi + O(1/\sqrt{N})$. For $N = 2$ the difference is exactly given by a factor of $\sqrt{2}$ as pointed out in Ref. [8].

The practical difference between the two protocols is, of course, insignificant. Nevertheless, it is interesting to see how it arises, as generalizations of this trick will be useful later. In the relevant two dimensional subspace for a given j , we can study the state on the Bloch sphere, where we take the north pole to be the initial state $|+\rangle$. The traditional goal is to evolve to the state $|j\rangle$ located near the south pole, and the Hamiltonian of Eq. (58) follows the obvious path that connects them. However, the ability to add in a Hamiltonian of arbitrary strength proportional to $|+\rangle\langle +|$ is equivalent to being able to do arbitrarily fast rotations around the vertical axis. Therefore, the set of points on a circle of constant latitude should all be regarded as a single point, and the optimal protocol involves choosing at each time the correct longitude so that the evolution southwards is greatest. In particular, the protocol need not arrive at $|j\rangle$ but may end at any of the other points of similar latitude, which the optimal protocol does.

The Farhi and Gutmann protocol [1] does achieve a more general goal: mainly given an oracle Hamiltonian $H = \pi|m\rangle\langle m|$, where the marked state $|m\rangle$ is arbitrary, evolve into the marked state (in a time that depends only on the overlap of the marked with the initial state). Our protocol essentially preassumes that the marked state is always a computational basis state. However, if our goal is to identify the Hamiltonian, then producing a copy of the marked state is only useful if the set of possible marked states is orthogonal, in which case we may assume that they belong to the computational basis.

IV. ORACLE INTERROGATION

We now turn our attention to the Hamiltonian oracle version of Oracle Interrogation [7], where the oracle has a n -bit string which can be queried one bit at a time, and the goal is to output the complete n -bit string. The problem is important as it serves as an upper bound on all problems where the goal is to output some function of the n -bit string.

We shall also briefly examine the XOR problem, where the goal is simply to output the XOR of the above n bits. In both the discrete and continuous oracle setting, this problem is nearly as hard as outputting the entire n -bit string.

A. Problem definition

Fix an integer $n \geq 1$, let $N = 2^n$, and define

$$\mathcal{A} = \text{span}\{|x\rangle \text{ for } x \in \{0,1\}^n\}, \quad (59)$$

$$\mathcal{M} = \text{span}\{|j,k\rangle \text{ for } j \in \{0\} \cup [n], k \in \{0,1\}\}. \quad (60)$$

We also introduce the final output spaces as $\mathcal{M}' = \mathcal{A}$ for oracle interrogation and $\mathcal{M}'_{\text{XOR}} = \text{span}\{|0\rangle, |1\rangle\}$ for the XOR problem. On these spaces define

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_x |x\rangle, \quad (61)$$

$$O = \sum_{x,j,k} (-1)^{x_j+k} |x\rangle\langle x|_{\mathcal{A}} \otimes |j,k\rangle\langle j,k|_{\mathcal{M}}, \quad (62)$$

$$H = \frac{\pi}{2} O, \quad (63)$$

$$\Pi_x = N|x\rangle\langle x|_{\mathcal{A}} \otimes |x\rangle\langle x|_{\mathcal{M}'}, \quad (64)$$

$$\Pi_{x,\text{XOR}} = N|x\rangle\langle x|_{\mathcal{A}} \otimes |\text{XOR}(x)\rangle\langle \text{XOR}(x)|_{\mathcal{M}'_{\text{XOR}}}, \quad (65)$$

where x ranges over the n -bit strings, $j = 0, \dots, n$ and $k \in \{0, 1\}$. We use the notation x_j to denote the j th bit of x , and define $x_0 = 0$. We also use $\text{XOR}(x)$ to denote the XOR of the n bits of x . The answer verification operators for oracle interrogation are $\{\Pi_x$ for $x \in \{0, 1\}^n\}$ whereas for the XOR problem they are $\{\Pi_{x,\text{XOR}}$ for $x \in \{0, 1\}^n\}$, otherwise the problems are identical.

Though the oracle O may look somewhat peculiar, it can be thought of as the regular oracle that applies a phase $(-1)^{x_j}$ to query state $|j\rangle$, followed by the σ_z Pauli operator on the last qubit. Since this operation is entirely on the message side, and could equally well be applied by Bob before or after the query, and therefore offers no extra computational power. As usual, Bob can also request a null query on the state $|0\rangle$.

In the continuous case, the extra bit k can be thought of as an arrow of time. For $k = 0$ the oracle applies one Hamiltonian and for $k = 1$ the oracle applies minus the same Hamiltonian. It is not clear whether one of these blocks is computationally equivalent to the complete Hamiltonian. This is an interesting open question. Unfortunately, the symmetrization approach to studying the oracle requires both blocks.

The normalization of H is chosen so that $e^{-iH} = -iO$, and hence the query time for the Hamiltonian oracle problem is a lower bound on the number of queries for the discrete oracle problem. The normalization does have the unfortunate property that at time $t = 1/2$ one can solve the $n = 1$ case exactly. However, the unitary $e^{-iH/2}$ is equivalent to performing the identity for a hidden zero bit, and applying phases of $\pm i$ for the hidden one bit, and these operations cannot simulate the standard one bit query.

B. Symmetrization

The natural symmetry group of these oracle problems is $G = (\mathbb{Z}_2)^n \rtimes S_n$, with a multiplication rule given by $(x', s')(x, s) = (x' \oplus s'(x), s's)$ where $s \in S_n$ and x is an n -bit binary string. The action of s on x is given by permutation of the bits.

The group G has a set of representations defined by

$$R_{\mathcal{A}}(x, s)|y\rangle_{\mathcal{A}} = |x \oplus s(y)\rangle_{\mathcal{A}}, \quad (66)$$

$$R_{\mathcal{M}}(x, s)|j, k\rangle_{\mathcal{M}} = |s(j), x_{s(j)} \oplus k\rangle_{\mathcal{M}}, \quad (67)$$

$$R_{\mathcal{M}'}(x, s)|y\rangle_{\mathcal{M}'} = |x \oplus s(y)\rangle_{\mathcal{M}'}, \quad (68)$$

$$R_{\mathcal{M}'_{\text{XOR}}}(x, s)|k\rangle_{\mathcal{M}'_{\text{XOR}}} = |\text{XOR}(x) \oplus k\rangle_{\mathcal{M}'_{\text{XOR}}}. \quad (69)$$

With these definitions, both oracle problems are compatible with G .

We begin the symmetrization by describing the most general positive operator ρ on \mathcal{A} that is G -invariant. We shall be working in the Hadamard basis for \mathcal{A} defined by

$$|\tilde{x}\rangle_{\mathcal{A}} = H^{\otimes n}|x\rangle_{\mathcal{A}}, \quad (70)$$

where H is the qubit Hadamard operator. In this basis, the representation $R_{\mathcal{A}}$ acts by

$$R_{\mathcal{A}}(x, s)|\tilde{y}\rangle = (-1)^{|x \oplus s(y)|} |\widetilde{s(y)}\rangle, \quad (71)$$

where $|x|$ denotes the Hamming weight. Invariance under G implies that $\langle \tilde{x}|\rho|\tilde{y}\rangle = \langle \tilde{x}|R_{\mathcal{A}}(g^{-1})\rho R_{\mathcal{A}}(g)|\tilde{y}\rangle$. Using elements of the form $g = (x', 1)$ we see that $\langle \tilde{x}|\rho|\tilde{y}\rangle = 0$ for $x \neq y$. Furthermore, using $g = (1, s)$ we see that $\langle \tilde{x}|\rho|\tilde{x}\rangle$ depends only on the Hamming weight of x . We can therefore write the most general G -invariant ρ as

$$\rho = \sum_{j=0}^n a_j^2 \left(\frac{1}{\binom{n}{j}} \sum_{|x|=j} |\tilde{x}\rangle\langle \tilde{x}| \right). \quad (72)$$

The normalization is chosen so that $\text{Tr}[\rho] = 1$ implies $\sum_j a_j^2 = 1$ and therefore the vector (a_0, \dots, a_n) is a point on the unit sphere S^n embedded in \mathbb{R}^{n+1} . Positivity of ρ requires $a_j^2 \geq 0$, which in turn requires a_j to be real. A unique set of ρ matrices can be generated by restricting to $a_j \geq 0$ for all j .

We now turn to the symmetrization of $\tilde{\rho}$. As G acts by permutation on \mathcal{M} , we can use the results of Section II C which provide us with a decomposition of the most general $\tilde{\rho}$ as

$$\tilde{\rho} = \sum_{j=0}^n \sum_{k=0}^1 \sigma_{j,k} \otimes |j, k\rangle\langle j, k|_{\mathcal{M}}, \quad (73)$$

where $\sigma_{0,0}$ and $\sigma_{0,1}$ must be G -invariant and the restriction on the remaining σ matrices is discussed below. We expand

$$\sigma_{0,k} = \sum_{j=0}^n \zeta_{j,k} \left(\frac{1}{\binom{n}{j}} \sum_{|x|=j} |\tilde{x}\rangle\langle \tilde{x}| \right). \quad (74)$$

As the evolution will only depend on the sum $\sigma_{0,0} + \sigma_{0,1}$ (i.e., they both correspond to null queries), it will be

convenient to define $\zeta_j = \zeta_{j,0} + \zeta_{j,1}$, which are required to be non-negative.

The remaining matrices are all related to each other by $\sigma_{j,k} = R_A(g)\sigma_{1,0}R_A(g^{-1})$ for any $g \in G$ such that $R_{\mathcal{M}}(g)|1,0\rangle_{\mathcal{M}} = |j,k\rangle_{\mathcal{M}}$. In particular, $\sigma_{1,0}$ must be invariant under the subgroup H of G that leaves $|1,0\rangle_{\mathcal{M}}$ invariant. We can write $H = (Z_2)^{n-1} \rtimes S_{n-1}$.

From Eq. (72) we see that \mathcal{A} decomposes into $n+1$ irreps of G given by $\text{span}\{|\tilde{x}\rangle \text{ for } |x| = j\}$ for $j = 0, \dots, n$. The $j=0$ and $j=n$ irreps are both one dimensional and therefore will also be irreps of H . Under the restriction to the subgroup H , the other irreps each split into two. An irrep of vectors with Hamming weight j will split into the vectors that have a zero in the first slot (which will be an irrep of H consisting of Hamming weight j vectors), and the vectors that have a one in the first slot (which will be an irrep of H consisting of Hamming weight $j-1$ vectors). In total, we end up with two copies of each of the n irreps. Each pair of irreps can share off diagonal elements but otherwise the matrix must be block diagonal. Therefore the most general H -invariant operator on \mathcal{A} has the form

$$\sigma_{1,0} = \sum_{j=0}^{n-1} \left[\begin{pmatrix} |\tilde{0}\rangle & |\tilde{1}\rangle \end{pmatrix} \begin{pmatrix} \alpha_j & \beta_j \\ \beta_j^* & \gamma_j \end{pmatrix} \begin{pmatrix} \langle \tilde{0}| \\ \langle \tilde{1}| \end{pmatrix} \right. \quad (75)$$

$$\left. \otimes \frac{1}{2n \binom{n-1}{j}} \sum_{\substack{z \in \{0,1\}^{n-1} \\ |z|=j}} |\tilde{z}\rangle \langle \tilde{z}| \right],$$

where we have decomposed \mathcal{A} into the first qubit and the remaining $n-1$ qubits. The notation means that, for instance, $|\tilde{0}\rangle \otimes |\tilde{z}\rangle = |\tilde{x}\rangle$ where x is the n -bit string obtained by concatenating 0 and z . Positivity of $\sigma_{1,0}$ is equivalent to $\alpha_j \geq 0$, $\gamma_j \geq 0$ and $\alpha_j \gamma_j \geq |\beta_j|^2$ for every j .

Note that the above form for an H -invariant $\sigma_{1,0}$ could also be obtained directly by noting that H -invariance implies that $\langle x|\sigma_{1,0}|y\rangle$ can depend only on the Hamming weight of the last $n-1$ bits of $x \oplus y$.

The normalizations above have been chosen in order to simplify the equation $\rho = \text{Tr}_{\mathcal{M}}[\tilde{\rho}]$ which is now equivalent to

$$a_j^2 = \begin{cases} \zeta_0 + \alpha_0 & j = 0, \\ \zeta_j + \alpha_j + \gamma_{j-1} & 0 < j < n, \\ \zeta_n + \gamma_{n-1} & j = n. \end{cases} \quad (76)$$

C. Boundary conditions

The initial condition is simply given by $a_0 = 1$ and $a_j = 0$ for $j > 0$. For the final probabilities of success, we note that after symmetrization, the probability of correctly outputting x or $\text{XOR}(x)$ is independent of the hidden string x , therefore we can replace the final mea-

surements by

$$\Pi = \sum_x |x\rangle \langle x|_{\mathcal{A}} \otimes |x\rangle \langle x|_{\mathcal{M}'} \quad (77)$$

$$\Pi_{\text{XOR}} = \sum_x |x\rangle \langle x|_{\mathcal{A}} \otimes |\text{XOR}(x)\rangle \langle \text{XOR}(x)|_{\mathcal{M}'_{\text{XOR}}} \quad (78)$$

for the oracle interrogation and XOR problems respectively. The final step is then a standard state discrimination problem dependent only on $\rho(T)$.

For oracle interrogation, $\rho(T)$ is proportional to the Gram matrix of the states to be distinguished. Since it is diagonal in the Hadamard basis, $\sqrt{\rho(T)}$ is also diagonal in the Hadamard basis and hence its diagonal elements in the computational basis are all equal. Just as in the Grover search case above, this implies [19, 20, 21] that the optimal measurement is the pretty good measurement and the success probability is given by

$$P_{\text{win}}(\rho(T)) = \frac{1}{N} \left(\text{Tr} \sqrt{\rho(T)} \right)^2 \quad (79)$$

$$= \frac{1}{N} \left(\sum_j \sqrt{\binom{n}{j}} a_j(T) \right)^2 = (\vec{a}(T) \cdot \vec{a}_f)^2.$$

where $\vec{a}(T) = (a_0(T), \dots, a_n(T))$ which involves the components of $\rho(T)$. The target vector \vec{a}_f with components

$$(\vec{a}_f)_j = \sqrt{\frac{1}{N} \binom{n}{j}} \quad (80)$$

has unit length, and so a zero error solution requires $\vec{a}(T) = \vec{a}_f$.

The last step in the XOR problem involves the state discrimination of two mixed states. As Bob has the purification of $\rho(T)$, we can write the joint state as $\sqrt{\rho(T)} \otimes I |\Phi\rangle$ where $|\Phi\rangle = \sum_x |x\rangle_{\mathcal{A}} \otimes |x\rangle_{\mathcal{M}'}$. The two states to discriminate are therefore given by

$$\eta_k = \text{Tr}_{\mathcal{A}} \left[P_k \otimes I \left(\sqrt{\rho(T)} \otimes I \right) |\Phi\rangle \langle \Phi| \left(\sqrt{\rho(T)} \otimes I \right) \right]$$

$$= \left(\sqrt{\rho(T)} P_k \sqrt{\rho(T)} \right)^T, \quad (81)$$

where $k \in \{0, 1\}$, P_k is the projector onto states $|x\rangle$ with $\text{XOR}(x) = k$, and the transpose is taken in the computational basis. The normalization is set to $\text{Tr}[\eta_k] = 1/2$ which is the a priori probability. Now we can use the result of Helstrom for two-state discrimination [22], so that

$$P_{\text{win}}(\rho(T)) = \frac{1}{2} \text{Tr}(\eta_0 + \eta_1 + |\eta_0 - \eta_1|) \quad (82)$$

$$= \frac{1}{2} + \frac{1}{2} \text{Tr} \left| \sqrt{\rho(T)} (P_0 - P_1) \sqrt{\rho(T)} \right|$$

$$= \frac{1}{2} + \frac{1}{2} \sum_{j=0}^n a_j(T) a_{n-j}(T),$$

where in the last step we use the fact that $P_0 - P_1 = \sigma_x^{\otimes n}$ in the Hadamard basis, and so the matrix inside the

absolute value is block diagonal with blocks pairing $|\tilde{x}\rangle$ and $|x \oplus 1 \cdots 1\rangle$.

From the above discussion we can see that the zero error XOR final states satisfy $a_j = a_{n-j}$ for all j . Furthermore if $a_j = 0$ for $j \geq n/2$ then $P_{win} \leq 1/2$ for both the XOR and oracle interrogation problems. In fact, we have for both problems

$$P_{win} \leq \frac{1}{2} + \sqrt{\sum_{j=\lfloor \frac{n}{2} \rfloor}^n a_j^2(T)}. \quad (83)$$

D. Discrete oracle dynamics

We shall only sketch the discrete oracle case here for comparison. From Eq. (8) we get the dynamics

$$\rho(t+1) = \sigma_{0,0}(t) + \sigma_{0,1}(t) + 2n [O_{1,0}\sigma_{1,0}(t)O_{1,0}^{-1}]_{sym}, \quad (84)$$

where $[\]_{sym}$ refers to the projection to the G -invariant subspace. The operator $O_{1,0}$ is the unitary realized when state $|1,0\rangle_{\mathcal{M}}$ is queried, and has the effect exchanging $\alpha_i \leftrightarrow \gamma_i$ and $\beta \leftrightarrow \beta^*$, leading to the equations

$$a_j^2(t+1) = \begin{cases} \zeta_0(t) + \gamma_0(t) & j = 0, \\ \zeta_j(t) + \gamma_j(t) + \alpha_{j-1}(t) & 0 < j < n, \\ \zeta_n(t) + \alpha_{n-1}(t) & j = n. \end{cases} \quad (85)$$

In combination with the constraint Eq. (76), one can see that at every step we can split $a_j^2(t)$ into three pieces: one which will get added into $a_{j+1}^2(t+1)$, one which will be added into $a_{j-1}^2(t+1)$ and one which will remain in $a_j^2(t+1)$. Inductively, we can prove that the set of achievable vectors after t queries satisfy $a_j = 0$ for $j > t$ but otherwise need only satisfy the normalization constraint $\sum_j a_j^2 = 1$.

In particular, this proves that for the XOR problem $P_{win} = 1/2$ for $T < n/2$ whereas $P_{win} = 1$ for $T = \lceil n/2 \rceil$, which is achieved as follows: for n even $a_{n/2}^2 = 1$ and the rest zero, for n odd $a_{(n\pm 1)/2}^2 = 1/2$ and the rest zero.

For oracle interrogation we see that an exact solution requires $T = n$. However, since most of the amplitude of the final vector \vec{a}_f is contained in the indices $a_{n/2 \pm O(\sqrt{n})}$ the problem can be solved to high accuracy by only correctly adjusting these components. This requires a query time $T = n/2 + O(\sqrt{n})$ reproducing the result of van Dam [7].

E. Continuous oracle dynamics

From Eq. (9) we get the dynamics

$$\frac{d\rho(t)}{dt} = -2ni [H_{1,0}\sigma_{1,0}(t) - \sigma_{1,0}(t)H_{1,0}]_{sym}, \quad (86)$$

where as before $[\]_{sym}$ is the projection onto the symmetric subspace and $H_{1,0} = \frac{\pi}{2} \sum_x (-1)^{x_1} |x\rangle\langle x|$. In each of the 2×2 blocks comprising $\sigma_{1,0}$, $H_{1,0}$ is proportional to the Pauli σ_x operator (as the blocks are in the Hadamard basis) and hence each block leads to a calculation of the form

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha_j & \beta_j \\ \beta_j^* & \gamma_j \end{pmatrix} - \begin{pmatrix} \alpha_j & \beta_j \\ \beta_j^* & \gamma_j \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -2i \operatorname{Im}[\beta_j] & \gamma_j - \alpha_j \\ \alpha_j - \gamma_j & 2i \operatorname{Im}[\beta_j] \end{pmatrix} \quad (87)$$

which leads to the differential equations

$$\frac{da_j^2(t)}{dt} = -\pi \begin{cases} \operatorname{Im} \beta_0(t) & j = 0, \\ \operatorname{Im} \beta_j(t) - \operatorname{Im} \beta_{j-1}(t) & 0 < j < n, \\ -\operatorname{Im} \beta_{n-1} & j = n. \end{cases} \quad (88)$$

Now we apply the constraints from the positivity of $\sigma_{1,0}$ which imply $|\operatorname{Im} \beta_j(t)| \leq \sqrt{\alpha_j(t)\gamma_j(t)}$. From Eq. (76) we also have $a_j^2 \leq \alpha_j + \gamma_{j-1}$ (with $\alpha_n = \gamma_{-1} = 0$). We can therefore write at every time

$$\operatorname{Im} \beta_j(t) = b_j(t)c_{j+1}(t)a_j(t)a_{j+1}(t), \quad (89)$$

where the new parameters represent Bob's degrees of freedom but must be consistent with the constraint $b_j^2(t) + c_j^2(t) \leq 1$ for $j = 0, \dots, n$. Canceling a factor of $a_j(t)$ we obtain

$$\frac{d}{dt} \vec{a}(t) = M(t) \vec{a}(t), \quad (90)$$

where $M(t)$ is the $(n+1) \times (n+1)$ real antisymmetric (as required by probability conservation) matrix which is zero everywhere except the entries one-off from the diagonal

$$M(t)_{j,j+1} = -M(t)_{j+1,j} = -\frac{\pi}{2} b_j(t)c_{j+1}(t) \quad (91)$$

for $j = 0, \dots, n-1$. An extra factor of $1/2$ appears in the above equation from the relation $\frac{da^2}{dt} = 2a \frac{da}{dt}$.

Note that in the transition to Eq. (90) we canceled factors of $a_j(t)$ which potentially could be zero. All this implies is that the derivative of $a_j(t)$ need not satisfy the above equation when $a_j = 0$. However, this is a set of measure zero, and a continuous evolution of \vec{a} will require that the above equation be satisfied at all times.

Let us rehash the current state of the problem. The vector $\vec{a}(t)$ indicates the state of the system (and hence Bob's knowledge of the hidden string) at a given time. Bob can affect this parameter by controlling the matrix $M(t)$ which he can modify at any time. The matrix $M(t)$ must have the form given by Eq. (91) with $b_j^2(t) + c_j^2(t) \leq 1$ but otherwise can be chosen arbitrarily. Bob must choose the parameters $\{b_j(t), c_j(t)\}$ to evolve from the initial condition of $\vec{a}(0) = (1, 0, \dots, 0)$ in order to maximize $\vec{a}(T) \cdot \vec{a}_f$ at some final time T and with

high probability solve the oracle interrogation problem. A similar end criterion was formulated above for the XOR problem.

Unfortunately, finding such an optimal evolution is still a difficult problem. We shall find below the optimal strategies for zero-error oracle interrogation for $n = 1$ and $n = 2$. The latter case is obtained by studying the geodesics of S^2 with a Riemannian metric. For $n > 2$ the metrics appear to be of Finsler type, and therefore beyond the scope of this paper. Nevertheless, we shall also prove a simple lower bound that will apply both to the oracle interrogation and XOR problems and will apply to bounded error solutions as well.

F. The $n = 1$ case

For $n = 1$ the differential equation reads

$$\frac{d}{dt} \begin{pmatrix} a_0(t) \\ a_1(t) \end{pmatrix} = -\frac{\pi}{2} b_0(t) c_1(t) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} a_0(t) \\ a_1(t) \end{pmatrix} \quad (92)$$

with constraints $b_0^2 \leq 1$ and $c_1^2 \leq 1$ (note that c_0 and b_1 do not appear anywhere in the equation). The initial condition is $\vec{a}(0) = (1, 0)$ and the final vector for zero error oracle interrogation is $\vec{a}(T) = \vec{a}_f = (1, 1)/\sqrt{2}$.

The optimal algorithm is to choose $b_0(t) = c_1(t) = 1$ at all times, in which case we obtain the evolution

$$\begin{pmatrix} a_0(t) \\ a_1(t) \end{pmatrix} = \begin{pmatrix} \cos \pi t/2 \\ \sin \pi t/2 \end{pmatrix}. \quad (93)$$

The minimum time required to arrive at the zero error final point is $T = 1/2$.

G. The $n = 2$ case

For $n = 2$ the differential equation reads

$$\frac{d}{dt} \begin{pmatrix} a_0(t) \\ a_1(t) \\ a_2(t) \end{pmatrix} = \frac{\pi}{2} \begin{pmatrix} 0 & -w_1(t) & 0 \\ w_1(t) & 0 & -w_2(t) \\ 0 & w_2(t) & 0 \end{pmatrix} \begin{pmatrix} a_0(t) \\ a_1(t) \\ a_2(t) \end{pmatrix} \quad (94)$$

with $w_1 = -b_0 c_1$ and $w_2 = -b_1 c_2$, which are constrained by $w_1^2 + w_2^2 \leq 1$.

If we position the unit sphere so that the vector $(0, 1, 0)$ corresponds with the north pole, then effectively, Bob can perform any rotation around an axis that lies on the equator and at a speed less than or equal to $\pi/2$ radians per unit time. Rotations around other axes can only be generated as composite rotations.

Thus far we have restricted ourselves to vectors \vec{a} from the intersection of the non-negative cone with the unit sphere. However we can now lift the restriction and allow vectors from the entire unit sphere. The only consequence of this is that we must identify points that differ by changes of sign, as the real state $\rho(t)$ depends only on $a_i^2(t)$. We now have to consider two possible starting

points and eight possible zero-error ending points. The symmetry (reflections north-south and east-west) reduces the set of inequivalent pairs to only two: starting from $(1, 0, 0)$ and ending at either $(1, \sqrt{2}, 1)/2$ or $(-1, \sqrt{2}, 1)/2$. Note that the paths that connect to the latter point would still be allowed under the restriction to the non-negative cone, but would have required a “bounce” on a boundary.

We shall now reformulate the problem in the language of differential geometry, where the sphere will acquire a non-round metric constructed so that the shortest distance between two points is equal to the minimum query time that is needed to evolve from one point to the other. The notation used below will follow the conventions adopted in general relativity.

It will be convenient to work in polar coordinates

$$a_0 = \sin \theta \cos \phi, \quad (95)$$

$$a_1 = \cos \theta, \quad (96)$$

$$a_2 = \sin \theta \sin \phi, \quad (97)$$

where the initial condition is now $\theta = \pi/2$, $\phi = 0$ and the final points are $\theta = \pi/4$, $\phi = \pi/2 \pm \pi/4$. Associated to this basis we have the coordinate (unnormalized) basis for the tangent space

$$e_\theta = (\cos \theta \cos \phi, -\sin \theta, \cos \theta \sin \phi), \quad (98)$$

$$e_\phi = (-\sin \theta \sin \phi, 0, \sin \theta \cos \phi), \quad (99)$$

At any given time, the set of possible velocity vectors depends on the current position and the Bob controlled parameters w_1, w_2 and is given by

$$\frac{\pi}{2} \begin{pmatrix} 0 & -w_1 & 0 \\ w_1 & 0 & -w_2 \\ 0 & w_2 & 0 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \frac{\pi}{2} \left(w_\theta e_\theta + \frac{w_\phi}{\tan \theta} e_\phi \right), \quad (100)$$

where we introduced

$$w_\theta = w_2 \sin \phi - w_1 \cos \phi, \quad (101)$$

$$w_\phi = w_2 \cos \phi + w_1 \sin \phi. \quad (102)$$

The constraint $w_1^2 + w_2^2 \leq 1$ is equivalent to $w_\theta^2 + w_\phi^2 \leq 1$. It is always optimal for Bob to choose the magnitude of the velocity to be as large as possible consistent with the chosen direction, and hence the inequality constraint will always be saturated. This produces a set of velocity vectors that correspond to unit velocity. The same set can be generated by the metric

$$ds^2 = \frac{4}{\pi^2} (d\theta^2 + \tan^2 \theta d\phi^2) \quad (103)$$

and therefore the distance assigned to a curve by this metric will be equal to the time it would take Bob to evolve the system through that curve. One is now left with the problem of finding curves of minimal distance on the surface with the above metric.

Strictly speaking the metric is ill defined on the equator, where our initial point lies. One can instead study

curves that begin at $\theta = \pi/2 - \epsilon$ and $\phi = 0$ and then bound the distance of these points to the equator. The resulting total distance in the limit $\epsilon \rightarrow 0$, however, will be the same as will be derived below by ignoring the divergence at the equator.

We can also describe the metric by its non-zero components $g_{\theta\theta} = \frac{4}{\pi^2}$ and $g_{\phi\phi} = \frac{4}{\pi^2} \tan^2 \theta$. The Christoffel symbols are defined by

$$\Gamma_{\mu\nu}^\lambda = \frac{1}{2} g^{\lambda\delta} (g_{\mu\delta,\nu} + g_{\delta\nu,\mu} - g_{\mu\nu,\delta}) \quad (104)$$

and therefore the non-zero symbols for our metric are given by

$$\Gamma_{\phi\phi}^\theta = -\frac{1}{2} \frac{\partial}{\partial \theta} \tan^2 \theta = -\frac{\sin \theta}{\cos^3 \theta}, \quad (105)$$

$$\Gamma_{\theta\phi}^\phi = \Gamma_{\phi\theta}^\phi = \frac{1}{2 \tan^2 \theta} \frac{\partial}{\partial \theta} \tan^2 \theta = \frac{1}{\sin \theta \cos \theta}. \quad (106)$$

The geodesic equation is

$$\frac{dv^\lambda}{dt} = -\Gamma_{\mu\nu}^\lambda v^\mu v^\nu, \quad (107)$$

where v is the velocity vector. Using dots for time derivatives the geodesic differential equations for our metric can be written as

$$\ddot{\theta} = \frac{\sin \theta}{\cos^3 \theta} \dot{\phi}^2, \quad (108)$$

$$\ddot{\phi} = \frac{-2}{\sin \theta \cos \theta} \dot{\theta} \dot{\phi}. \quad (109)$$

The second equation is solved by

$$\dot{\phi} = \pm \frac{\pi \tan \theta_0}{2 \tan^2 \theta}, \quad (110)$$

where θ_0 is an arbitrary parameter whose form will become clear in a moment. The same equation can also be obtained directly by the variation of the action with respect to ϕ . The geodesic equation also implies the conservation of the total speed, which we normalize to one

$$1 = g_{\theta\theta} \dot{\theta}^2 + g_{\phi\phi} \dot{\phi}^2. \quad (111)$$

We can now combine the two previous equations to obtain a differential equation for θ

$$\dot{\theta} = \pm \frac{\pi}{2} \sqrt{1 - \frac{\tan^2 \theta_0}{\tan^2 \theta}}, \quad (112)$$

where the meaning of θ_0 becomes clear: it defines the maximum height of the geodesic curve. The differential equation is solved by

$$\begin{aligned} \frac{\pi}{2} t &= \pm \int \frac{\cos(\theta_0) \sin \theta d\theta}{\sqrt{\cos^2 \theta_0 \sin^2 \theta - \sin^2 \theta_0 \cos^2 \theta}} \\ &= \mp \int \frac{\cos \theta_0 d(\cos \theta)}{\sqrt{\cos^2 \theta_0 - \cos^2 \theta}} \\ &= \cos \theta_0 \arcsin \left(\frac{\cos \theta}{\cos \theta_0} \right), \end{aligned} \quad (113)$$

where in the last step we have chosen our constant and sign so that $t = 0$ corresponds to the initial condition of $\theta = \pi/2$, and as time increases we move north.

Now we turn to the differential equation for ϕ which can be obtained by substituting the above solution into Eq. (110)

$$\begin{aligned} \dot{\phi} &= \pm \frac{\pi \tan \theta_0}{2} \left(\frac{1}{1 - \cos^2 \theta} - 1 \right) \\ &= \pm \frac{\pi \tan \theta_0}{2} \left(\frac{1}{1 - \cos^2 \theta_0 \sin^2 \frac{\pi t}{2 \cos \theta_0}} - 1 \right). \end{aligned} \quad (114)$$

Using the derivative

$$\begin{aligned} \frac{d}{ds} \arctan(\sin \theta_0 \tan s) &= \frac{\sin \theta_0}{\cos^2 s} [1 + \sin^2 \theta_0 \tan^2 s]^{-1} \\ &= \frac{\sin \theta_0}{1 - \cos^2 \theta_0 \sin^2 s} \end{aligned} \quad (115)$$

we obtain

$$\begin{aligned} \phi &= -\frac{\pi t \tan \theta_0}{2} + \arctan \left(\sin \theta_0 \tan \frac{\pi t}{2 \cos \theta_0} \right) \\ &= -\sin \theta_0 \arcsin \left(\frac{\cos \theta}{\cos \theta_0} \right) + \arctan \left(\frac{\sin \theta_0 \frac{\cos \theta}{\cos \theta_0}}{\sqrt{1 - \frac{\cos^2 \theta}{\cos^2 \theta_0}}} \right) \end{aligned} \quad (116)$$

with a choice of the additive constant and sign so that $\phi = 0$ at $t = 0$, and ϕ increases with time. Unfortunately, solving for the constant θ_0 seems to require solving a transcendental equation, and therefore the calculation needs to be completed numerically.

Of course there are many geodesics that connect the points that we are interested in. Before proceeding with a numerical solution, we must ensure that we are examining the shortest geodesic.

The geodesics all start at the equator, rise up to some height $\cos \theta_0$, and then fall back again to the equator so that the curve is symmetric around the apex. During the transition from $\theta = \pi/2$ to $\theta = \theta_0$ we effect the following increases:

$$\Delta t = \cos \theta_0, \quad (117)$$

$$\Delta \phi = \frac{\pi}{2} (1 - \sin \theta_0). \quad (118)$$

Also note that if we remove the $\sin \theta_0$ factor from inside the arctan we increase the right-hand side of Eq. (116). Without that factor however, the arctan is equivalent to and arcsin and so we have

$$\phi \leq (1 - \sin \theta_0) \arcsin \left(\frac{\cos \theta}{\cos \theta_0} \right). \quad (119)$$

We learn two things from the above observations. First, we learn that on the way up, $\phi \leq (1 - 1/\sqrt{2})\pi/2 \leq \pi/4$ at $\theta = \pi/4$ so that we must pass the apex at least once before arriving at the zero-error solution. Second, we need a solution with $\theta_0 \leq \pi/4$ and hence the time to

climb to the apex and return to the equator is at least $2/\sqrt{2} > 1$ which is more time than it takes to query the two bits separately. Therefore the optimal solution must rise to the apex once, and arrive at either $\phi = \pi/4$ or $\phi = 3\pi/4$ on the way down. The time of arrival for such a trip is

$$T = 2 \cos \theta_0 \left(1 - \frac{1}{\pi} \arcsin \left(\frac{\cos \theta}{\cos \theta_0} \right) \right), \quad (120)$$

which increases as $\cos \theta_0$ gets larger. Since a geodesic to $\phi = 3\pi/4$ will require a larger $\cos \theta_0$ than one to $\phi = \pi/4$ we have proven that the shortest path to a zero error point arrives at $\phi = \pi/4$ after crossing through the apex exactly once. The total increase in ϕ over such a path is given by twice the right hand side of Eq. (118) minus the right hand side of Eq. (116). Substituting into this equation $\theta = \pi/4$ and $\phi = \pi/4$ we can numerically solve for $\cos \theta_0 \simeq 0.7477$. Using this value in the above equation we find that the query time needed to exactly solve the $n = 2$ case of oracle interrogation is

$$T \simeq 0.9052. \quad (121)$$

That is, only about 90% of the time it would require to query both bits separately.

H. Lower bound

To conclude we shall prove a weak but fairly simple lower bound on the query time needed to solve the Hamiltonian oracles for XOR and oracle interrogation even in the bounded error setting.

From the discrete case we learn that in general amplitude moves from the variables a_j with low values of j to the ones with high values of j . We also know that after only t queries, the variables a_j with $j > t$ are zero. Though this no longer holds in the continuous case, it does motivate the study of the variables

$$A_j = \sqrt{\sum_{k=j}^n a_k^2}. \quad (122)$$

From the dynamical of Eq. (90) we have for $j > 0$

$$\begin{aligned} \frac{dA_j^2(t)}{dt} &= 2 \sum_{k=j}^n a_k(t) \frac{da_k(t)}{dt} \\ &= \pi b_{j-1}(t) c_j(t) a_j(t) a_{j-1}(t). \end{aligned} \quad (123)$$

Using $A_j \geq a_j$, $b_{j-1} \leq 1$ and $c_j \leq 1$ we obtain

$$\frac{dA_j(t)}{dt} \leq \frac{\pi}{2} A_{j-1}(t). \quad (124)$$

An inductive solution can be constructed because we know that for all time $A_0(t) = 1$ by conservation of probability, and the remaining initial conditions are $A_j(0) = 0$ for $j > 0$. Therefore

$$A_j(t) \leq \frac{1}{j!} \left(\frac{\pi t}{2} \right)^j. \quad (125)$$

In particular, we know from Eq. (83) that we can relate the probability of success to the above variables by $P_{win}(T) \leq \frac{1}{2} + A_{\lfloor n/2 \rfloor}(T)$. Therefore, the query time needed to solve the Hamiltonian versions of XOR and oracle interrogation with bounded error is at least

$$\begin{aligned} T &\geq \frac{2}{\pi} \left(\left\lfloor \frac{n}{2} \right\rfloor! \right)^{1/\lfloor \frac{n}{2} \rfloor} \left| P_{win}(T) - \frac{1}{2} \right|^{1/\lfloor \frac{n}{2} \rfloor} \\ &\geq \frac{n}{\pi e} + \Omega(1) \simeq 0.117n. \end{aligned} \quad (126)$$

The bound is likely weak in the continuous case, and certainly weak as a lower bound of the discrete case. Nevertheless, it captures the essential $O(n)$ scaling. The main open question is: can similar continuous methods be used to prove lower bounds for new problems?

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